

Oxydation of Methanol to Formaldehyde on V₂O₅ Investigated by Density Functional Theory

P. Boulet, F. Gilardoni, J. Weber, H. Chermette, A. Baiker, J.-C.
Volta

published in

Modern Methods and Algorithms of Quantum Chemistry,
J. Grotendorst (Ed.), John von Neumann Institute for Computing,
Jülich, NIC Series, Vol. 2, ISBN 3-00-005746-3, p. 4, 2000.

© 2000 by John von Neumann Institute for Computing

Permission to make digital or hard copies of portions of this work for personal or classroom use is granted provided that the copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise requires prior specific permission by the publisher mentioned above.

<http://www.fz-juelich.de/nic-series/>

Oxydation Of Methanol to Formaldehyde On V_2O_5 Investigated By Density Functional Theory.

P. Boulet^{1,2,4}, F. Gilardoni², J. Weber², H. Chermette^{1,2}, A. Baiker³ and J.-C. Volta⁴

¹ *Laboratoire de chimie physique théorique, Université Claude Bernard Lyon 1, Bât 210, 43 Bld du 11 novembre 1918, 69622 Villeurbanne cedex.*

² *Département de Chimie-Physique, Université de Genève, 30 Quai E-Ansermet, CH-1211 Genève 4.*

³ *Laboratory of Technical Chemistry, ETH Zentrum CNB, CH-8092 Zürich, Switzerland.*

⁴ *Institut de Recherches sur la Catalyse, CNRS, 2 av. Albert Einstein, 69626 Villeurbanne cedex.*

As a precursor to materials of industrial interest formaldehyde is one of the most widely used chemicals. One way to obtain formaldehyde is to dehydrogenate methanol on vanadium oxide-based catalysts. Lots of work remain to be accomplished to understand the chemical processes of the reaction.

In this poster, we present the adsorption of methanol and propose a mechanism for the mild oxidation.

